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| | | |
|--------------|-----------|--|
| NEWS | 1 | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS | 2 | "Ask CAS" for self-help around the clock |
| NEWS | 3 JAN 27 | Source of Registration (SR) information in REGISTRY updated and searchable |
| NEWS | 4 JAN 27 | A new search aid, the Company Name Thesaurus, available in CA/CAplus |
| NEWS | 5 FEB 05 | German (DE) application and patent publication number format changes |
| NEWS | 6 MAR 03 | MEDLINE and LMEDLINE reloaded |
| NEWS | 7 MAR 03 | MEDLINE file segment of TOXCENTER reloaded |
| NEWS | 8 MAR 03 | FRANCEPAT now available on STN |
| NEWS | 9 MAR 29 | Pharmaceutical Substances (PS) now available on STN |
| NEWS | 10 MAR 29 | WPIVF now available on STN |
| NEWS | 11 MAR 29 | New monthly current-awareness alert (SDI) frequency in RAPRA |
| NEWS | 12 APR 26 | PRQMT: New display field available |
| NEWS | 13 APR 26 | IFIPAT/IFIUDB/IFICDB: New super search and display field available |
| NEWS | 14 APR 26 | LITALERT now available on STN |
| NEWS | 15 APR 27 | NLDB: New search and display fields available |
| NEWS | 16 May 10 | PROUSDDR now available on STN |
| NEWS | 17 May 19 | PROUSDDR: One FREE connect hour, per account, in both May and June 2004 |
| NEWS | 18 May 12 | EXTEND option available in structure searching |
| NEWS | 19 May 12 | Polymer links for the POLYLINK command completed in REGISTRY |
| NEWS | 20 May 17 | FRFULL now available on STN |
| NEWS | 21 May 27 | STN User Update to be held June 7 and June 8 at the SLA 2004 Conference |
| NEWS | 22 May 27 | New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus |
| NEWS | 23 May 27 | CAplus super roles and document types searchable in REGISTRY |
| NEWS | 24 May 27 | Explore APOLLIT with free connect time in June 2004 |
| NEWS EXPRESS | | MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004 |
| NEWS HOURS | | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | | General Internet Information |
| NEWS LOGIN | | Welcome Banner and News Items |
| NEWS PHONE | | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | | CAS World Wide Web Site (general information) |

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 16 JUN 2004 HIGHEST RN 694434-66-7
DICTIONARY FILE UPDATES: 16 JUN 2004 HIGHEST RN 694434-66-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

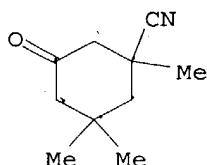
```
=> isophoronenitrile/cn  
ISOPHORONENITRILE IS NOT A RECOGNIZED COMMAND  
The previous command name entered was not recognized by the system.  
For a list of commands available to you in the current file, enter  
"HELP COMMANDS" at an arrow prompt (>).
```

=> s isophoronenitrile/cn
L1 1 ISOPHORONENITRILE/CN

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 7027-11-4 REGISTRY
CN Cyclohexanecarbonitrile, 1,3,3-trimethyl-5-oxo- (7CI, 8CI, 9CI) (CA INDEX
NAME)
OTHER NAMES:
CN 3-Cyano-3,5,5-trimethylcyclohexanone
CN 3-Oxo-1,5,5-trimethylcyclohexanecarbonitrile
CN Isophoronenitrile
CN NSC 171143

FS 3D CONCORD
DR 144975-27-9, 78948-79-5
MF C10 H15 N O
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPIUS, CASREACT, CHEMCATS, CHEMLIST,
RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); FORM (Formation,
nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process);
RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: PREP (Preparation);
RACT (Reactant or reagent)
RL.NP Roles from non-patents: BIOL (Biological study); MSC (Miscellaneous);
PREP (Preparation); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

88 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
88 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> s isophorone/cn
L2 1 ISOPHORONE/CN

=> d

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 78-59-1 REGISTRY
CN 2-Cyclohexen-1-one, 3,5,5-trimethyl- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN α -Isophoron
CN α -Isophorone
CN 1,1,3-Trimethyl-3-cyclohexene-5-one
CN 1,5,5-Trimethyl-3-oxocyclohexene
CN 1-Cyclohexen-3-one, 1,5,5-trimethyl-
CN 3,5,5-Trimethyl-2-cyclohexen-1-one
CN 3,5,5-Trimethyl-2-cyclohexene-1-one
CN 3,5,5-Trimethyl-2-cyclohexenone
CN Isoacetophorone
CN Isoforon
CN Isophoron
CN **Isophorone**

CN NSC 403657
 CN NSC 4881
 FS 3D CONCORD
 MF C9 H14 O
 CI COM

LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, DIPPR*, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USPAT2, USPATFULL, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

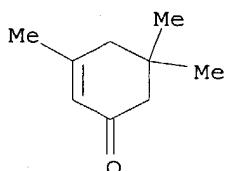
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.P Roles for non-specific derivatives from patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2503 REFERENCES IN FILE CA (1907 TO DATE)
 20 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 2506 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 23 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

| | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|---------------------|------------------|
| => file casreact | | |
| COST IN U.S. DOLLARS | | |
| FULL ESTIMATED COST | 14.50 | 14.71 |

FILE 'CASREACT' ENTERED AT 15:13:02 ON 17 JUN 2004
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FILE CONTENT:1840 - 13 Jun 2004 VOL 140 ISS 24

*
* CASREACT now has more than 8 million reactions *
*

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

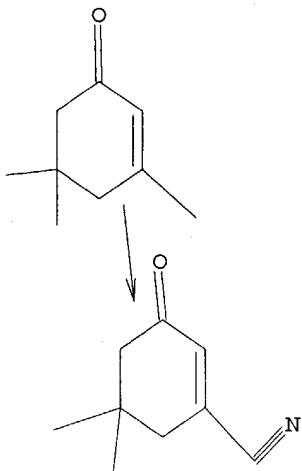
Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=>
Uploading C:\Program Files\Stnexp\Queries\10701513.str

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L3

10/458135

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SAMPLE SEARCH INITIATED 15:13:41 FILE 'CASREACT'
SCREENING COMPLETE - 2 REACTIONS TO VERIFY FROM 2 DOCUMENTS

100.0% DONE 2 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 2 TO 124
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3 (0 REACTIONS)

=> s L3 full
FULL SEARCH INITIATED 15:13:52 FILE 'CASREACT'
SCREENING COMPLETE - 8 REACTIONS TO VERIFY FROM 6 DOCUMENTS

100.0% DONE 8 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

L5 0 SEA SSS FUL L3 (0 REACTIONS)

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
SESSION
FULL ESTIMATED COST 103.98 118.69

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FILE COVERS 1907 - 17 Jun 2004 VOL 140 ISS 25
FILE LAST UPDATED: 16 Jun 2004 (20040616/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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(FILE 'HOME' ENTERED AT 15:09:39 ON 17 JUN 2004)

FILE 'REGISTRY' ENTERED AT 15:10:00 ON 17 JUN 2004
L1 1 S ISOPHORONENITRILE/CN
L2 1 S ISOPHORONE/CN

FILE 'CASREACT' ENTERED AT 15:13:02 ON 17 JUN 2004

L3 STRUCTURE uploaded
 L4 0 S L3
 L5 0 S L3 FULL

FILE 'CAPLUS' ENTERED AT 15:15:24 ON 17 JUN 2004

=> s L1
 L6 88 L1

=> s L2
 L7 2508 L2

=> s L6 and L7
 L8 28 L6 AND L7

=> s L8 and (HCN or hydrogen cyanide)
 22796 HCN
 823229 HYDROGEN
 75403 CYANIDE
 8638 HYDROGEN CYANIDE
 (HYDROGEN (W) CYANIDE)
 L9 18 L8 AND (HCN OR HYDROGEN CYANIDE)

=> s L9 and ?oxide
 2400861 ?OXIDE
 L10 7 L9 AND ?OXIDE

=> d L8 1-28 ibib abs

L8 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2004:386596 CAPLUS

DOCUMENT NUMBER: 140:391385
 TITLE: Regioselective hydrocyanation process for the calcium oxide-catalyzed preparation of isophorone nitrile from hydrogen cyanide and isophorone
 INVENTOR(S): Kunsmann-Keitel, Dagmar; Braun, Gerold; Muenster, Ingo; Mundinger, Klaus; Scherhag, Gunter; Siegel, Wolfgang
 PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
 SOURCE: Eur. Pat. Appl., 5 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|--------------------|----------|
| EP 1418172 | A2 | 20040512 | EP 2003-25652 | 20031107 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| DE 10251680 | A1 | 20040519 | DE 2002-10251680 | 20021107 |
| JP 2004155785 | A2 | 20040603 | JP 2003-375444 | 20031105 |
| US 2004092761 | A1 | 20040513 | US 2003-701513 | 20031106 |
| PRIORITY APPLN. INFO.: AB | | | DE 2002-10251680 A | 20021107 |
| A regioselective hydrocyanation process for the calcium oxide-catalyzed preparation of isophorone nitrile from hydrogen cyanide and isophorone is presented in which the calcium oxide regioselective hydrocyanation catalyst has a BET surface area of >1.5 m ² /g. | | | | |

L8 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2000:96029 CAPLUS
 DOCUMENT NUMBER: 132:124501
 TITLE: Hydrocyanation process and catalyst for the preparation of 3-cyano-3,5,5-trimethylcyclohexanone from isophorone and hydrogen cyanide
 INVENTOR(S): Fischer, Jakob; Siegel, Wolfgang; Bomm, Volker; Fischer, Martin; Mundinger, Klaus
 PATENT ASSIGNEE(S): BASF A.-G., Germany
 SOURCE: U.S., 4 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|------------------|----------|
| US 6022988 | A | 20000208 | US 1999-372062 | 19990811 |
| DE 19836474 | A1 | 20000217 | DE 1998-19836474 | 19980812 |
| EP 985659 | A1 | 20000315 | EP 1999-115469 | 19990805 |
| EP 985659 | B1 | 20031029 | | |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

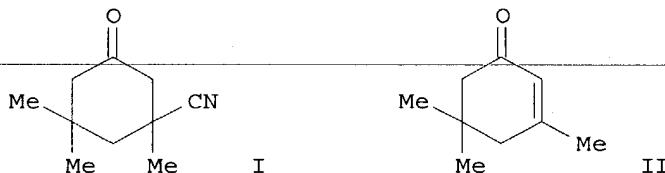
PRIORITY APPLN. INFO.: DE 1998-19836474 A 19980812
 AB 3-Cyano-3,5,5-trimethylcyclohexanone is prepared in high yield and selectivity by reacting isophorone with hydrogen cyanide at 80-220° in the presence of the betaine catalyst 1,3-dimethylimidazolium-4-carboxylate

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1999:662214 CAPLUS
 DOCUMENT NUMBER: 132:49772
 TITLE: Synthesis of 3H-labeled 2-hydroxy-N-[(1,3,3-trimethyl-[4,5,6-3H]cyclohexyl)methyl]-5-azidobenzamide, a photoaffinity analog of an influenza fusion inhibitor
 AUTHOR(S): Dischino, Douglas D.; Cianci, Christopher; Krystal, Mark; Meanwell, Nicholas A.; Morimoto, Hiromi; Pearce, Bradley C.; Williams, Philip; Yu, Kuo-Long
 CORPORATE SOURCE: The Richard L. Gelb Center for Research and Development, Bristol-Myers Squibb Company, Wallingford, CT, 06492-7660, USA
 SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1999), 42(10), 965-974
 CODEN: JLCRD4; ISSN: 0362-4803
 PUBLISHER: John Wiley & Sons Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The title compound was prepared by tritiation of a mixture of N-(tert.-butoxycarbonyl)-1,3,3-trimethylcyclohex-4- and -5-enylmethylamine via T2 and Pd/C, followed by coupling of the deprotected tritiated α with 5-azidoacetylsalicylic acid chloride, followed by deprotection target compound was obtained with a radiochem. purity > 99% and a ϵ activity of 63 Ci/mmol.
 REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE RECORD. ALL CITATIONS AVAILABLE IN THE

L8 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1995:907770 CAPLUS
 DOCUMENT NUMBER: 123:313436
 TITLE: Process for the preparation of 3-cyano-3,5,5-trimethylcyclohexanone [isophorone nitrile]
 INVENTOR(S): Mundinger, Klaus; Laqua, Gerhard; Witzel, Tom; Merger, Franz
 PATENT ASSIGNEE(S): BASF A.-G., Germany
 SOURCE: Eur. Pat. Appl., 8 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|----------|
| EP 671384 | A1 | 19950913 | EP 1995-102923 | 19950302 |
| EP 671384 | B1 | 19991103 | | |
| R: BE, DE, FR, GB | | | | |
| DE 4407487 | A1 | 19950914 | DE 1994-4407487 | 19940307 |
| US 5516928 | A | 19960514 | US 1995-395322 | 19950228 |
| PRIORITY APPLN. INFO.: | | | DE 1994-4407487 | 19940307 |
| OTHER SOURCE(S): | CASREACT 123:313436; MARPAT 123:313436 | | | |
| GI | | | | |



AB The title compound (I), an intermediate for the monomer isophoronediamine, is prepared by a method using ~~improved~~ catalysts. Thus, isophorone (II) reacts with HCN to give I, at 80-180° and 0.5-20 bar, in the presence of an ammonium salt catalyst R1R2R3R4N⁺ X⁻ [R1-R4 = C1-18 alkyl, C5-8 cycloalkyl, aryl, C7-18 aralkyl, C2-18 hydroxyalkyl; X = OCO₂H, or OCO₂R where R = C1-8 alkyl]. For example, a mixture of 3 mol HCN and 1.5 mol II was added over 60 min to a mixture of 4.5 mol II and 30 mmol Me₄N⁺ MeOCO₂⁻ at 120°. Acidification with 3.5 g 85% H₃PO₄ and distillation at 0.1 mbar gave I in 99% or 96.2% yield (based on unreacted II or fed HCN, resp.). In comparison, use of Et₄N⁺ CN⁻ catalyst gave 89.6% yield based on fed HCN. Also used as catalysts were BuMe₃N⁺ MeOCO₂⁻, and Et₃MeN⁺ MeOCO₂⁻, which gave similar results.

L8 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1995:401307 CAPLUS
 DOCUMENT NUMBER: 122:160152
 TITLE: Process for producing amines by reductive amination in the presence of a cobalt catalyst.
 INVENTOR(S): Furutani, Atsushi; Hibi, Takuo; Yamamoto, Michio; Tanaka, Kazuyuki; Tada, Kazuhiro; Fukao, Masami; Suzukamo, Gohfu

PATENT ASSIGNEE(S) : Sumitomo Chemical Co., Ltd., Japan
 SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------|
| EP 623585 | A1 | 19941109 | EP 1994-300903 | 19940208 |
| EP 623585 | B1 | 19980422 | | |
| R: BE, DE, FR, GB | | | | |
| JP 07101910 | A2 | 19950418 | JP 1994-6466 | 19940125 |
| CA 2115024 | AA | 19941028 | CA 1994-2115024 | 19940204 |
| US 5589596 | A | 19961231 | US 1994-194328 | 19940208 |
| PRIORITY APPLN. INFO.: | | | JP 1993-101074 | 19930427 |
| | | | JP 1993-180248 | 19930721 |
| | | | JP 1993-180249 | 19930721 |
| | | | JP 1993-196041 | 19930806 |
| | | | JP 1993-197339 | 19930809 |

OTHER SOURCE(S) : CASREACT 122:160152

AB A process is disclosed for producing amines by reductive amination of cyclic ketones or their imino derivs., characterized by use of a cobalt catalyst containing an alkaline earth metal carbonate and/or lanthanum oxide.

The

new catalysts give high yields, are highly active, and are usable on a com. scale. For example, an aqueous solution of Co and Cu nitrates was treated with Ca carbonate, heated to 80°, and treated with aqueous Na carbonate to give a precipitate, which was retreated with aqueous Na carbonate, dried, heated

in N at 320°, cooled, granulated, and hydrogenated at 280° to give a catalyst. 3-Cyano-3,5,5-trimethylcyclohexanone was then passed with MeOH and liquid NH₃ through a first reactor containing active C at 24° and 150 kg/cm²G to give the imine derivative in 97.7% yield. This was passed through the above catalyst in a second reactor at 121° and the same pressure to give 3-aminomethyl-3,5,5-trimethylcyclohexylamine (I) in 99.4% yield, plus minor amts. of 2 byproducts. A comparison catalyst without the Cu nitrate or the Ca carbonate gave only 90.7% yield of I in the second step, with 5.8% 3-aminomethyl-3,5,5-trimethylcyclohexyl alc. and 3.2% 1,3,3-trimethyl-6-azabicyclo[3.2.1]octane as byproducts.

L8 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:630393 CAPLUS

DOCUMENT NUMBER: 121:230393

TITLE: Preparation of amines from cyclic ketones.

INVENTOR(S) : Furutani, Atsushi; Hibi, Takuo; Yamamoto, Michio; Suzukamo, Gohfu

PATENT ASSIGNEE(S) : Sumitomo Chemical Company, Ltd., Japan

SOURCE: Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|----------|
| EP 611137 | A1 | 19940817 | EP 1994-300915 | 19940208 |

| | | | | |
|------------------------|----|----------|-----------------|----------|
| EP 611137 | B1 | 19960424 | | |
| R: BE, DE, FR, GB | | | | |
| JP 06285370 | A2 | 19941011 | JP 1993-324532 | 19931222 |
| JP 07228562 | A2 | 19950829 | JP 1994-303 | 19940106 |
| CA 2115025 | AA | 19940809 | CA 1994-2115025 | 19940204 |
| US 5395972 | A | 19950307 | US 1994-194329 | 19940208 |
| PRIORITY APPLN. INFO.: | | | JP 1993-20134 | 19930208 |
| | | | JP 1993-319593 | 19931220 |

OTHER SOURCE(S): CASREACT 121:230393

AB Cyclic ketones were reacted with NH₃ in the presence of active C to produce imino derivs. which were reacted with H in the presence of a hydrogenation catalyst to give the corresponding amines. Thus, 3-cyano-3,5,5-trimethylcyclohexanone, MeOH, and NH₃ were fed to the first of a series of 2 connected reactors and H was added to the second reactor, the first packed with active C and the second packed with Co on silica. The temperature of the first reactor was 20° and that of the second was 114°; reactor pressure was 70 kg/cm²G. Product 3-aminomethyl-3,5,5-trimethylcyclohexylamine was formed in 94.9% yield.

L8 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:511943 CAPLUS

DOCUMENT NUMBER: 121:111943

TITLE: Purification of 3-cyano-3,5,5-trimethyl-1-cyclohexanone

INVENTOR(S): Terasawa, Shoichi; Yamamoto, Masahiro

PATENT ASSIGNEE(S): Asahi Chemical Ind, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 06065183 | A2 | 19940308 | JP 1992-225631 | 19920825 |

PRIORITY APPLN. INFO.: JP 1992-225631 19920825

AB The title compound (I), prepared by the base-catalyzed addition reaction of HCN with isophorone, is purified by adding an inert compound having a higher b.p. than I and compatible with I, removing the basic catalyst, high-boiling impurities, and the inert compound in a thin-film evaporator, and separating isophorone from I in a distillation column. A reaction product

(180

g) containing isophorone 18.02, I 80.9, high-boiling impurities 1.0, and NaOH 0.08% was mixed with 3 g polyethylene glycol (II; mol. weight 400) and fed to a thin-film evaporator to give 177.3 g fraction containing 18.2% isophorone and 81.8% I (for separation by distillation) and 5.7 g fraction containing II 53,

isophorone 3, and I 10%.

L8 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:511942 CAPLUS

DOCUMENT NUMBER: 121:111942

TITLE: Purification of 3-cyano-3,5,5-trimethyl-1-cyclohexanone

INVENTOR(S): Terasawa, Shoichi; Kondo, Yoshikimi

PATENT ASSIGNEE(S): Asahi Chemical Ind, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 06065182 | A2 | 19940308 | JP 1992-215834 | 19920813 |

PRIORITY APPLN. INFO.: JP 1992-160927 19920619
 AB The title compound (I), prepared by the alkali-catalyzed addition reaction of HCN with isophorone is purified by neutralizing the catalyst with an acid and distilling the mixture. A reaction mixture containing I 60.5, isophorone 38, and KOH 0.30 mol was neutralized with H₂SO₄ and distilled (540 parts) in vacuo to give 226 parts distillate containing 12.7% I and 87.3% isophorone and 286 parts crystalline fraction containing 99.5% I.

L8 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:670685 CAPLUS
 DOCUMENT NUMBER: 119:270685
 TITLE: Process for the continuous preparation of 3-cyano-3,5,5-trimethylcyclohexanone
 INVENTOR(S): Pander, Hans Joachim; Siegel, Hardo; Woerz, Otto
 PATENT ASSIGNEE(S): BASF A.-G., Germany
 SOURCE: Eur. Pat. Appl., 6 pp.
 CODEN: EPXXDW

DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------|------|----------|-----------------|----------|
| EP 554786 | A1 | 19930811 | EP 1993-101250 | 19930128 |
| EP 554786 | B1 | 19951129 | | |
| R: BE, DE, FR, GB, NL | | | | |
| DE 4203456 | A1 | 19930812 | DE 1992-4203456 | 19920207 |
| US 5254711 | A | 19931019 | US 1993-14171 | 19930205 |
| JP 06122667 | A2 | 19940506 | JP 1993-18562 | 19930205 |
| JP 3241472 | B2 | 20011225 | | |

PRIORITY APPLN. INFO.: DE 1992-4203456 A 19920207

OTHER SOURCE(S): CASREACT 119:270685
 AB The title process comprises condensation of isophorone with HCN in a 2-stage flow reactor system comprising an initial stage wherein complete mixing is provided and a second stage wherein mixing is suppressed. Thus, operation at 150° in both stages gave 96.5% the title compound

L8 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:652567 CAPLUS
 DOCUMENT NUMBER: 119:252567
 TITLE: Process for the preparation of 3-cyano-3,5,5-trimethylcyclohexanone
 INVENTOR(S): Woodbury, Richard P.; Thunberg, Jon C.; Vankouwenberg, Steven P.; Begonis, Walter B.
 PATENT ASSIGNEE(S): Hampshire Chemical Corp., USA
 SOURCE: U.S., 10 pp.
 CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| US 5235089 | A | 19930810 | US 1992-843867 | 19920227 |
| AU 9333783 | A1 | 19930902 | AU 1993-33783 | 19930225 |
| AU 660765 | B2 | 19950706 | | |
| CA 2090555 | AA | 19930828 | CA 1993-2090555 | 19930226 |
| EP 558332 | A1 | 19930901 | EP 1993-301451 | 19930226 |
| EP 558332 | B1 | 19960529 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, PT, SE | | | | |
| JP 06016612 | A2 | 19940125 | JP 1993-61314 | 19930226 |
| AT 138642 | E | 19960615 | AT 1993-301451 | 19930226 |
| ES 2088225 | T3 | 19960801 | ES 1993-301451 | 19930226 |
| PRIORITY APPLN. INFO.: | | | US 1992-843867 | 19920227 |

AB The title process giving title compound with high yield and low impurity comprises reacting isophorone with HCN in the presence of LiCN catalyst at 80-115° while maintaining the HCN at a controlled rate (to prevent the generation of free LiOH, diisophorone, its nitrile derivs., and HCN polymer); and adding an acid selected from malic acid, oxalic acid, sulfuric acid, and phosphoric acid to precipitate the Li salt.

L8 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:233534 CAPLUS

DOCUMENT NUMBER: 118:233534

TITLE: Catalyst and process for the production of 3-cyano-3,5,5-trialkylcyclohexanone

INVENTOR(S): Forguy, Christian; Goetz, Frederick J.; Graeber, Edward L.; Lindstrom, Michael J.

PATENT ASSIGNEE(S): Elf Atochem North America, Inc., USA

SOURCE: U.S., 4 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| US 5183915 | A | 19930202 | US 1992-846364 | 19920305 |
| EP 558799 | A2 | 19930908 | EP 1992-117471 | 19921013 |
| EP 558799 | A3 | 19950215 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE | | | | |
| CA 2080646 | AA | 19930906 | CA 1992-2080646 | 19921015 |
| JP 05294918 | A2 | 19931109 | JP 1992-314450 | 19921030 |
| CN 1075954 | A | 19930908 | CN 1992-112660 | 19921103 |
| PRIORITY APPLN. INFO.: | | | US 1992-846364 | 19920305 |

OTHER SOURCE(S): MARPAT 118:233534

AB Title compound is prepared by reaction of 3,5,5-tris(C1-4 alkyl)cyclohexanone with HCN in the absence of H₂O and in the presence of quaternary ammonium- or phosphonium cyanide catalyst at 900-120° and 1-3 bar pressure. Isophorone and Et₄N⁺CN⁻ was heated to 105° followed by addition of HCN after which the temperature was increased to 112° and kept at 1102 for 1 h with stirring to give 3-cyclohexa-3,5,5-trimethylcyclohexanone.

L8 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:59336 CAPLUS

DOCUMENT NUMBER: 118:59336
 TITLE: Preparation of 3-cyano-3,5,5-trimethylcyclohexanone
 INVENTOR(S): Tabei, Nobuaki; Mizuno, Tadashi; Okamura, Haruki
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------|
| JP 04253948 | A2 | 19920909 | JP 1991-15229 | 19910206 |
| PRIORITY APPLN. INFO.: | | | JP 1991-15229 | 19910206 |

OTHER SOURCE(S): CASREACT 118:59336; MARPAT 118:59336
 AB The title compound (I) is prepared by treating isophorone (II) with HCN in the presence of R₂N:C(NR₁₂)₂ (III; R₁, R₂ = H, C₁₋₄ alkyl). A mixture of II and III (R₁ = Me, R₂ = H) was treated dropwise with HCN at 105° over 3 h, then settled at 105° for 0.5 h to give 90.6% I.

L8 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1993:21969 CAPLUS
 DOCUMENT NUMBER: 118:21969
 TITLE: Preparation of 3-cyano-3,5,5-trimethylcyclohexanone
 INVENTOR(S): Terasawa, Shoichi; Yamamoto, Tadatsugu
 PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------|
| JP 04279558 | A2 | 19921005 | JP 1991-4451 | 19910118 |
| PRIORITY APPLN. INFO.: | | | JP 1991-4451 | 19910118 |

AB The title compound (I) is prepared by treating isophorone with HCN in the presence of basic catalysts and water. A mixture of isophorone and aqueous NaOH was treated dropwise with HCN, then stirred at 170° to give I in 100% selectivity at 47.6% conversion.

L8 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1992:570855 CAPLUS
 DOCUMENT NUMBER: 117:170855
 TITLE: Preparation of 3-cyano-3,5,5-trimethylcyclohexanone
 INVENTOR(S): Terasawa, Shoichi; Yamamoto, Tadatsugu
 PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|------|-----------------|------|
|------------|------|------|-----------------|------|

JP 04164057 A2 19920609 JP 1990-285816 19901025
 PRIORITY APPLN. INFO.: JP 1990-285816 19901025
 OTHER SOURCE(S): CASREACT 117:170855
 AB The title compds. (I), useful as material for 1-amino-3-aminomethyl-3,5,5-trimethylcyclohexane and 1-isocyanato-3-(isocyanatomethyl)-3,5,5-trimethylcyclohexane, is prepared by treating isophorone (II) with HCN in 1,3-dimethyl-2-imidazolidinone (III) in the presence of basic catalysts. A mixture of II and K₂CO₃ in III was treated dropwise with HCN at 110° over 4 h, then treated at 110° for 1 h to give I in 94% selectivity at 88% conversion.

L8 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:492650 CAPLUS
 DOCUMENT NUMBER: 117:92650
 TITLE: Manufacture of 3-cyano-3,5,5-trimethylcyclohexanone
 INVENTOR(S): Terasawa, Shoichi; Yamamoto, Tadatsugu
 PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|----------|
| JP 04112862 | A2 | 19920414 | JP 1990-232491 | 19900904 |
| PRIORITY APPLN. INFO.: | | | JP 1990-232491 | 19900904 |
| AB | Title compound (I) is manufactured from isophorone and HCN at 60-160° in Me ₂ SO and/or DMF over a base catalyst. Thus, treating 1 mol isophorone with 1 mol HCN in Me ₂ SO in the presence of K ₂ CO ₃ at 110° gave 85% I vs. 41% in ethylene glycol. | | | |

L8 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:425974 CAPLUS
 DOCUMENT NUMBER: 117:25974
 TITLE: Preparation of bis-(3-cyano-3,5,5-trimethylcyclohexylidene)azine and its conversion to 3-(aminomethyl)-3,5,5-trimethylcyclohexylamine
 INVENTOR(S): Huthmacher, Klaus; Schmitt, Hermann
 PATENT ASSIGNEE(S): Degussa A.-G., Germany
 SOURCE: Eur. Pat. Appl., 11 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| EP 482347 | A2 | 19920429 | EP 1991-115713 | 19910917 |
| EP 482347 | A3 | 19920819 | | |
| EP 482347 | B1 | 19930609 | | |
| R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL | | | | |
| DE 4033609 | A1 | 19920507 | DE 1990-4033609 | 19901023 |
| DE 4033609 | C2 | 19920910 | | |
| DE 4119577 | A1 | 19921217 | DE 1991-4119577 | 19910614 |
| AT 90335 | E | 19930615 | AT 1991-115713 | 19910917 |
| ES 2059008 | T3 | 19941101 | ES 1991-115713 | 19910917 |

| | | | | |
|------------------------|----|----------|-----------------|----------|
| JP 04264057 | A2 | 19920918 | JP 1991-273630 | 19911022 |
| US 5166396 | A | 19921124 | US 1991-785323 | 19911023 |
| US 5166444 | A | 19921124 | US 1992-848390 | 19920309 |
| PRIORITY APPLN. INFO.: | | | DE 1990-4033609 | 19901023 |
| | | | DE 1991-4119577 | 19910614 |
| | | | EP 1991-115713 | 19910917 |
| | | | US 1991-785323 | 19911023 |

OTHER SOURCE(S): CASREACT 117:25974

AB The title azine, prepared in 92.7% yield from 1,3,3-trimethyl-5-oxocyclohexanecarbonitrile and N₂H₄ in MeOH, was hydrogenated in MeOH-NH₃ in the presence of Raney Ni and CoCl₂ to give 91.2% title amine.

L8 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1991:514033 CAPLUS
 DOCUMENT NUMBER: 115:114033
 TITLE: Process for the preparation of 1,3,3-trimethyl-5-oxo-cyclohexanecarbonitrile
 INVENTOR(S): Huthmacher, Klaus; Schmitt, Hermann
 PATENT ASSIGNEE(S): Degussa A.-G., Germany
 SOURCE: Eur. Pat. Appl., 7 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------------------------|------|----------|-----------------|----------|
| EP 433615 | A1 | 19910626 | EP 1990-120672 | 19901029 |
| EP 433615 | B1 | 19931208 | | |
| R: BE, CH, DE, ES, FR, GB, IT, LI, NL | | | | |
| DE 3942371 | A1 | 19910627 | DE 1989-3942371 | 19891221 |
| DE 3942371 | C2 | 19920521 | | |
| ES 2060893 | T3 | 19941201 | ES 1990-120672 | 19901029 |
| US 5091554 | A | 19920225 | US 1990-622786 | 19901205 |
| JP 06128214 | A2 | 19940510 | JP 1990-402612 | 19901217 |
| JP 07091256 | B4 | 19951004 | | |
| CA 2032667 | AA | 19910622 | CA 1990-2032667 | 19901219 |
| CA 2032667 | C | 19960917 | | |

PRIORITY APPLN. INFO.: DE 1989-3942371 19891221

OTHER SOURCE(S): CASREACT 115:114033

AB A process for the preparation of 1,3,3-trimethyl-5-oxo-1-cyclohexanecarbonitrile (I) comprises the addition of HCN to isophorone in the presence of an alkali compound (LiOH) as catalyst at 100-160°; 0.0005-5 mol% catalyst are used with resp. to isophorone. HCN (40.5 g) was added to a mixture of isophorone (345 g) and LiOH (0.8 g) at 135° to give 89.1% I.

L8 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1991:470990 CAPLUS
 DOCUMENT NUMBER: 115:70990
 TITLE: Process for the preparation of 3-cyano-3,5,5-trimethylcyclohexanone by addition of hydrogen cyanide to isophorone
 INVENTOR(S): Thunberg, Jon C.; Begonis, Walter B.
 PATENT ASSIGNEE(S): W. R. Grace and Co., USA
 SOURCE: U.S., 7 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|----------|
| US 5011968 | A | 19910430 | US 1990-475051 | 19900206 |
| CA 2034640 | AA | 19910807 | CA 1991-2034640 | 19910121 |

PRIORITY APPLN. INFO.: US 1990-475051 19900206

AB The title compound (I), i.e. isophorone nitrile, is prepared by (a) reacting isophorone (II) with HCN in the presence of a quaternary ammonium hydroxide in a molar ratio of II:HCN:catalyst of (.apprx.2.00-3.00):1.00:(0.005-0.01) at a least 110°; (b) decomposing the remaining catalyst by heating the reaction mixture at .apprx.110-150°; (c) sparging with an inert gas at 100-200° to remove the catalyst decomposition product) and (d) acidifying the mixture with an acid and sparging with an inert gas to eliminate residual HCN. Thus, 172 lb II was charged via vacuum to a reactor of an apparatus (illustrated therein), N was introduced to break the vacuum, II was heated to 110°, 1.11 lb of 25% aqueous Me4N+OH- was added, and HCN was added, and the reaction was allowed to proceed to give I.

L8 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:448914 CAPLUS
 DOCUMENT NUMBER: 115:48914
 TITLE: Preparation of 3-cyano-3,5,5'-trimethyl-1-cyclohexanone from isophorone and an alkaline cyanide
 INVENTOR(S): Pontoglio, Enrico; Parodi, Sandro
 PATENT ASSIGNEE(S): Caffaro S.p.A., Italy
 SOURCE: Eur. Pat. Appl., 5 pp.
 CODEN: EPXXDW

DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

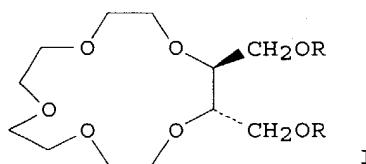
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------------------|------|----------|-----------------|----------|
| EP 425806 | A1 | 19910508 | EP 1990-117995 | 19900919 |
| EP 425806 | B1 | 19940601 | | |
| R: CH, DE, ES, FR, LI, NL | | | | |
| ES 2054185 | T3 | 19940801 | ES 1990-117995 | 19900919 |
| US 5142090 | A | 19920825 | US 1990-585240 | 19900920 |
| JP 03153656 | A2 | 19910701 | JP 1990-298751 | 19901102 |

PRIORITY APPLN. INFO.: IT 1989-22246 19891102

AB The title compound (I), which is used as a hardener for epoxy resins and as a monomer for polyurethane and polyamide resins, is prepared by reaction of isophorone (II) with an equivalent amount of an alkaline cyanide in a homogeneous

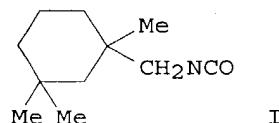
water/organic solvent solution at 20° to reflux temperature while maintaining a pH between 14-8 by a gradual addition of an inorg. acid during the reaction. Thus, II 553, DMF 600, and an aqueous NaCN 600 parts were heated at 90-92° with stirring while adding 85% H3PO4 and after 2 h the feeding of the acid was stopped and the temperature was raised to 104-105° allowing the reaction to complete for another 2 h. The reaction mixture was brought to pH 5.5 with 85% H3PO4 and the upper layer containing I was removed and then distilled on a Vigreux column to give 78% I of 97% purity.

L8 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1989:439343 CAPLUS
 DOCUMENT NUMBER: 111:39343
 TITLE: Applications of phase-transfer catalysis. Part 45.
 Enantioselective phase-transfer catalysis by optically active crown ethers
 AUTHOR(S): Dehmlow, Eckehard V.; Sauerbier, Christiane
 CORPORATE SOURCE: Fak. Chem., Univ. Bielefeld, Bielefeld, D-4800/1, Fed. Rep. Ger.
 SOURCE: Liebigs Annalen der Chemie (1989), (2), 181-5
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 111:39343
 GI



AB Chiral crown ethers I ($R = H, R_1CO; R_1 = Ph$, substituted Ph) were prepared as chiral phase-transfer catalysts. I induced asymmetry in the epoxidation of alkenones and in their reaction with $HOCMe_2CN$. The maximum enantiomeric excess, 45%, was obtained in the reaction of (E)- $PhCH:CHCOPh$ with $HOCMe_2CN$ in the presence of I ($R = 2,4-Cl_2C_6H_3CO$).

L8 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1987:190539 CAPLUS
 DOCUMENT NUMBER: 106:190539
 TITLE: Guinea pig pulmonary response to sensitization by five preformed monoisocyanate-ovalbumin conjugates
 AUTHOR(S): De Ceaurriz, Jacques; Ducos, Philippe; Micillino, Jean Claude; Gaudin, Rene; Cavelier, Claude
 CORPORATE SOURCE: Inst. Natl. Rech. Sec., Vandoeuvre, 54500, Fr.
 SOURCE: Toxicology (1987), 43(1), 93-101
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The ability of 5 dissimilar monoisocyanates conjugated to ovalbumin (OA) as a carrier protein to induce pulmonary hypersensitivity towards the hapten specific component was assessed by using a previously described

method based on the determination of a respiratory index (RI) in the guinea pig.

The test chemical included p-tolyl [622-58-2] and hexylmonoisocyanate [2525-62-4] (TMI and HMI), 4-isocyanatodiphenylmethane (IDM) [1823-37-6], 4-isocyanato-4'-methyldiphenylmethane (IMDM) [107997-84-2], and 1-isocyanatomethyl-1,3,3-trimethylcyclohexane (IMTC) (I) [107997-85-3]. Guinea pigs were exposed daily to an aerosol of the OA conjugate of each monoisocyanate up to ≤ 15 days. Increases in respiratory rate and/or respiratory collapse occurred in the guinea pigs exposed to TMI-OA and HMI-OA conjugates by days 9 and 15, with RI values of 155 and 177, resp.. The greatest mean RI values in guinea pigs exposed to IDM-OA, IMDM-OA, and IMTC-OA conjugates to day 15 were 20, 25, and 22, resp., and were not indicative of any pulmonary reaction. Guinea pigs exposed in parallel to each test conjugate did not exhibit any pulmonary reaction when they were exposed to OA on the challenge days. All these findings evidence pulmonary hypersensitivity as the result of exposure to TMI-OA and HMI-OA conjugates and suggest a high degree of conjugation and strong linkage of all the monoisocyanates with OA. The difference between the number of days to the onset of pulmonary reaction to TMI-OA and HMI-OA conjugates, and the lack of pulmonary reaction to IDM-OA, IMDM-OA, and IMTC-OA conjugates within the exptl. period suggest the influence of the nature of the haptic portion on the lapse of time required for pulmonary response to OA preformed conjugates and point to the possibility of discriminating between the allergenic potential of the test materials on this basis.

L8 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:442383 CAPLUS
 DOCUMENT NUMBER: 105:42383
 TITLE: 3-Cyano-3,5,5-trimethylcyclohexanone
 INVENTOR(S): Kondo, Kenji; Kosai, Hiroshi; Shidara, Hideo
 PATENT ASSIGNEE(S): Nippon Chemicals Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 61033157 | A2 | 19860217 | JP 1984-153231 | 19840725 |
| JP 05033217 | B4 | 19930519 | | |

PRIORITY APPLN. INFO.: JP 1984-153231 19840725

OTHER SOURCE(S): CASREACT 105:42383

AB The title compound (I), useful as epoxy resin hardener, material for elastomers, polyurethane paints, etc. (no data), was prepared by reaction of isophorone (II) and HCN over quaternary ammonium hydroxide or quaternary phosphonium hydroxide. Thus, HCN was added dropwise to mixture of II, Bu₄NOH, and H₂O with stirring at 110° for 3 h and the resulting mixture allowed to stand at 110° for 1 h to give 94.9% I based on HCN.

L8 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:442382 CAPLUS
 DOCUMENT NUMBER: 105:42382
 TITLE: 3-Cyano-3,5,5-trimethylcyclohexanone
 INVENTOR(S): Kondo, Kenji; Kosai, Hiroshi; Shidara, Hideo
 PATENT ASSIGNEE(S): Nippon Chemicals Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 61033158 | A2 | 19860217 | JP 1984-153233 | 19840725 |
| JP 04081583 | B4 | 19921224 | | |

PRIORITY APPLN. INFO.: JP 1984-153233 19840725

OTHER SOURCE(S): CASREACT 105:42382

GI For diagram(s), see printed CA Issue.

AB The title compound (I), useful as an epoxy resin hardener and material for elastomers, polyurethane paint, etc. (no data), was prepared by treating isophorone (II) with HCN in presence of diazabicycloalkenes III ($n = 2-11$, $m = 2-6$; both rings may have lower alkyl substituents). Thus, III was added dropwise to II containing 1,8-diazabicyclo[5.4.0]undecene with stirring at 110° for 3 h and the resulting mixture held at 110° for 1 h to give 96.5% I based on HCN.

L8 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:615625 CAPLUS

DOCUMENT NUMBER: 97:215625

TITLE: 3-Cyano-3,5,5-trimethylcyclohexanone

PATENT ASSIGNEE(S): Nitto Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

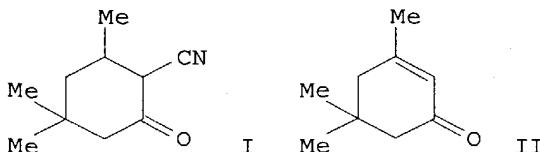
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 57116038 | A2 | 19820719 | JP 1981-2102 | 19810112 |
| JP 62005418 | B4 | 19870204 | | |

PRIORITY APPLN. INFO.: JP 1981-2102 19810112

GI



AB 3-Cyano-3,5,5-trimethylcyclohexanone (I) was prepared by reaction of isophorone (II) with HCN at $50-150^\circ$ in the presence of bases and glycols. Thus, 27.5 parts HCN was added to a mixture of II 351.5, Na₂CO₃ 2.7, and (HOCH₂)₂ 25 parts over 3 h at 100° to give, after 0.5 h, 92.9% I.

L8 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:597874 CAPLUS

DOCUMENT NUMBER: 97:197874
 TITLE: A novel conjugate hydrocyanation with titanium tetrachloride-tert-butyl isocyanide
 AUTHOR(S): Ito, Yoshihiko; Kato, Hidehito; Imai, Hiroshi; Saegusa, Takeo
 CORPORATE SOURCE: Fac. Eng., Kyoto Univ., Kyoto, 606, Japan
 SOURCE: Journal of the American Chemical Society (1982), 104(23), 6449-50
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 97:197874
 AB Conjugate hydrocyanation of α,β -unsatd. ketones is achieved in high yields by means of Me₃CNC with TiCl₄. Stereochem. of the conjugate hydrocyanation, which seems to be kinetically controlled, is demonstrated by the reactions of $\Delta^4(10)$ -octalin-3-one and 9-methyl- $\Delta^4(10)$ -octalin-3-one with TiCl₄-Me₃CNC, producing a 9:1 mixture of trans- and cis-10-cyanoctalin-3-one and a 7:3 mixture of trans- and cis-10-cyano-9-methyloctalin-3-one, resp. The conjugate hydrocyanation may be explained in terms of nucleophilic β -addition of Me₃CNC onto enone activated by TiCl₄, followed by β -elimination of tert-Bu cation to give β -cyanoketone. Conjugate hydrocyanations of α,β -unsatd. aldehyde and ester are also achieved in moderate yields by EtAlCl₂-Me₃CNC system and AlCl₃-Me₃CNC system, resp.

L8 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:514904 CAPLUS
 DOCUMENT NUMBER: 95:114904
 TITLE: 3-Cyano-3,5,5-trimethylcyclohexanone
 INVENTOR(S): Dubreux, Bernard
 PATENT ASSIGNEE(S): Produits Chimiques Ugine Kuhlmann, Fr.
 SOURCE: Eur. Pat. Appl., 10 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| EP 28179 | A1 | 19810506 | EP 1980-401455 | 19801010 |
| EP 28179 | B1 | 19821103 | | |
| R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE | | | | |
| FR 2468584 | A1 | 19810508 | FR 1979-26596 | 19791026 |
| FR 2468584 | B1 | 19840511 | | |
| US 4299775 | A | 19811110 | US 1980-185989 | 19800910 |
| JP 56071057 | A2 | 19810613 | JP 1980-133078 | 19800926 |
| JP 01047459 | B4 | 19891013 | | |
| AT 1746 | E | 19821115 | AT 1980-401455 | 19801010 |
| ES 496269 | A1 | 19811001 | ES 1980-496269 | 19801024 |
| PRIORITY APPLN. INFO.: | | | FR 1979-26596 | 19791026 |
| | | | EP 1980-401455 | 19801010 |

AB Isophorone reacted with metal cyanides and phase transfer agents to give the title compound (I). Thus, isophorone was heated with NaCN and Me(CH₂)₁₁N⁺(CH₂Ph)Me₂Br⁻ in water to yield I.

L8 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:138907 CAPLUS
 DOCUMENT NUMBER: 94:138907

TITLE: Stereochemistry. LII. Orbital verification of reaction stereochemistry. III. The effects of β -fluoro and β -cyano groups on the stereochemistry and kinetics of the reduction of cyclohexanones by lithium tri-tert-butoxyaluminum hydride

AUTHOR(S): Agami, C.; Kazakos, A.; Levisalles, J.; Sevin, A.
CORPORATE SOURCE: Lab. Chim. Org., Univ. Paris VI, Paris, 5, Fr.
SOURCE: Tetrahedron (1980), 36(20-21), 2977-81
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal
LANGUAGE: French

AB The effects were studied of β -fluoro and β -cyano groups on the kinetics and stereoselectivity of the reduction of ketones by $\text{Li}(\text{Me}_3\text{CO})_3\text{AlH}$ in the presence of and absence of cryptands, $\text{Me}(\text{CH}_2)_7\text{F}$, and MeCN . The results were discussed in relation to ab initio MO calcns. on the analogous carbonyl compds., $\text{H}_2\text{CRCH}_2\text{CHO}$ ($\text{R} = \text{H}, \text{F}, \text{CN}$).

L8 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1966:447345 CAPLUS
DOCUMENT NUMBER: 65:47345
ORIGINAL REFERENCE NO.: 65:8793d
TITLE: Synthesis of 3-cyano-3,5,5-trimethylcyclohexanone
PATENT ASSIGNEE(S): Scholven-Chemie A.-G.
SOURCE: 8 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|------|
| NL 6513694 | | 19660425 | NL | |

PRIORITY APPN. INFO.: DE 19641024

AB The title compound (I) can be prepared batch-wise or continuously from isophorone, HCN, and 10-1-10-3% alkaline catalyst at 110-200°. Thus, a mixture of 50 l. isophorone, 20 l. HCN, and 280 ml. 15% NaOH in MeOH is heated to 150°, 12.5 l. HCN is added in 4 hrs., and the mixture stirred 0.5 hr., washed with 0.65% HNO_3 solution to remove the alkaline catalyst, and distilled to yield 10.3 kg. isophorone, 96.2% I, and 1.6 kg. residue. A detailed description of a continuous process is given.

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L9 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN *Sample*
ACCESSION NUMBER: 2004:386596 CAPLUS
DOCUMENT NUMBER: 140:391385
TITLE: Regioselective hydrocyanation process for the calcium oxide-catalyzed preparation of isophorone nitrile from hydrogen cyanide and isophorone
INVENTOR(S): Kunsmann-Keitel, Dagmar; Braun, Gerold; Muenster, Ingo; Mundinger, Klaus; Scherhag, Gunter; Siegel, Wolfgang
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany
SOURCE: Eur. Pat. Appl., 5 pp.
DOCUMENT TYPE: Patent

LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|----------|
| EP 1418172 | A2 | 20040512 | EP 2003-25652 | 20031107 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| DE 10251680 | A1 | 20040519 | DE 2002-10251680 | 20021107 |
| JP 2004155785 | A2 | 20040603 | JP 2003-375444 | 20031105 |
| US 2004092761 | A1 | 20040513 | US 2003-701513 | 20031106 |

PRIORITY APPN. INFO.: DE 2002-10251680 A 20021107
 AB A regioselective hydrocyanation process for the calcium oxide-catalyzed preparation of isophorone nitrile from **hydrogen cyanide** and isophorone is presented in which the calcium oxide regioselective hydrocyanation catalyst has a BET surface area of >1.5 m²/g.

L9 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2000:96029 CAPLUS
 DOCUMENT NUMBER: 132:124501
 TITLE: Hydrocyanation process and catalyst for the preparation of 3-cyano-3,5,5-trimethylcyclohexanone from isophorone and **hydrogen cyanide**
 INVENTOR(S): Fischer, Jakob; Siegel, Wolfgang; Bomm, Volker;
 Fischer, Martin; Mundinger, Klaus
 PATENT ASSIGNEE(S): BASF A.-G., Germany
 SOURCE: U.S., 4 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|----------|
| US 6022988 | A | 20000208 | US 1999-372062 | 19990811 |
| DE 19836474 | A1 | 20000217 | DE 1998-19836474 | 19980812 |
| EP 985659 | A1 | 20000315 | EP 1999-115469 | 19990805 |
| EP 985659 | B1 | 20031029 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |

PRIORITY APPN. INFO.: DE 1998-19836474 A 19980812
 AB 3-Cyano-3,5,5-trimethylcyclohexanone is prepared in high yield and selectivity by reacting isophorone with **hydrogen cyanide** at 80-220° in the presence of the betaine catalyst/
1,3-dimethylimidazolium-4-carboxylate.

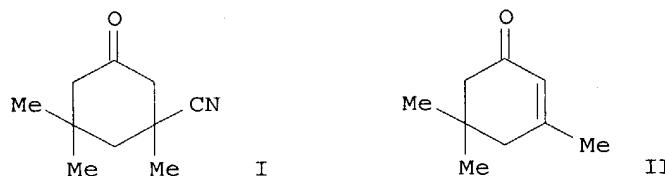
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1995:907770 CAPLUS
 DOCUMENT NUMBER: 123:313436
 TITLE: Process for the preparation of 3-cyano-3,5,5-trimethylcyclohexanone [isophorone nitrile]
 INVENTOR(S): Mundinger, Klaus; Laqua, Gerhard; Witzel, Tom; Merger, Franz
 PATENT ASSIGNEE(S): BASF A.-G., Germany
 SOURCE: Eur. Pat. Appl., 8 pp.

CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

1995

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|----------|
| EP 671384 | A1 | 19950913 | EP 1995-102923 | 19950302 |
| EP 671384 | B1 | 19991103 | | |
| R: BE, DE, FR, GB | | | | |
| DE 4407487 | A1 | 19950914 | DE 1994-4407487 | 19940307 |
| US 5516928 | A | 19960514 | US 1995-395322 | 19950228 |
| PRIORITY APPLN. INFO.: | | | DE 1994-4407487 | 19940307 |
| OTHER SOURCE(S): | CASREACT 123:313436; MARPAT 123:313436 | | | |
| GI | | | | |



AB The title compound (I), an intermediate for the monomer isophoronediamine, is prepared by a method using improved catalysts. Thus, isophorone (II) reacts with HCN to give I, at 80-180° and 0.5-20 bar, in the presence of an ammonium salt catalyst R1R2R3R4N+ X- [R1-R4 = C1-18 alkyl, C5-8 cycloalkyl, aryl, C7-18 aralkyl, C2-18 hydroxyalkyl; X = OCO2H, or OCO2R4 where R4 = C1-8 alkyl]. For example, a mixture of 3 mol HCN and 1.5 mol II was added over 60 min to a mixture of 4.5 mol II and 30 mmol Me4N+ MeOCO2- at 120°. Acidification with 3.5 g 85% H3PO4 and distillation at 0.1 mbar gave I in 99% or 96.2% yield (based on unreacted II or fed HCN, resp.). In comparison, use of Et4N+ CN- catalyst gave 89.6% yield based on fed HCN. Also used as catalysts were BuMe3N+ MeOCO2-, and Et3MeN+ MeOCO2-, which gave similar results.

L9 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1994:511943 CAPLUS
 DOCUMENT NUMBER: 121:111943
 TITLE: Purification of 3-cyano-3,5,5-trimethyl-1-cyclohexanone
 INVENTOR(S): Terasawa, Shoichi; Yamamoto, Masahiro
 PATENT ASSIGNEE(S): Asahi Chemical Ind, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 06065183 | A2 | 19940308 | JP 1992-225631 | 19920825 |

PRIORITY APPLN. INFO.: JP 1992-225631 19920825
 AB The title compound (I), prepared by the base-catalyzed addition reaction of HCN with isophorone, is purified by adding an inert compound having a higher b.p. than I and compatible with I, removing the basic catalyst, high-boiling impurities, and the inert compound in a thin-film evaporator, and separating isophorone from I in a distillation column. A reaction product

(180

g) containing isophorone 18.02, I 80.9, high-boiling impurities 1.0, and NaOH 0.08% was mixed with 3 g polyethylene glycol (II; mol. weight 400) and fed to a thin-film evaporator to give 177.3 g fraction containing 18.2% isophorone and 81.8% I (for separation by distillation) and 5.7 g fraction containing II 53,
 isophorone 3, and I 10%.

L9 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:511942 CAPLUS

DOCUMENT NUMBER: 121:111942

TITLE: Purification of 3-cyano-3,5,5-trimethyl-1-cyclohexanone

INVENTOR(S): Terasawa, Shoichi; Kondo, Yoshikimi

PATENT ASSIGNEE(S): Asahi Chemical Ind, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------|------|----------|-----------------|----------|
| JP 06065182 | A2 | 19940308 | JP 1992-215834 | 19920813 |

PRIORITY APPLN. INFO.: JP 1992-160924 19920619

AB The title compound (I), prepared by the alkali-catalyzed addition reaction of HCN with isophorone is purified by neutralizing the catalyst with an acid and distilling the mixture. A reaction mixture containing I 60.5, isophorone

38, and KOH 0.30 mol was neutralized with H₂SO₄ and distilled (540 parts) in vacuo to give 226 parts distillate containing 12.7% I and 87.3% isophorone and 286 parts crystalline fraction containing 99.5% I.

L9 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:670685 CAPLUS

DOCUMENT NUMBER: 119:270685

TITLE: Process for the continuous preparation of 3-cyano-3,5,5-trimethylcyclohexanone

INVENTOR(S): Pander, Hans Joachim; Siegel, Hardo; Woerz, Otto

PATENT ASSIGNEE(S): BASF A.-G., Germany

SOURCE: Eur. Pat. Appl., 6 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|----------|
| EP 554786 | A1 | 19930811 | EP 1993-101250 | 19930128 |
| EP 554786 | B1 | 19951129 | | |

R: BE, DE, FR, GB, NL

| | | | | |
|-------------|----|----------|-----------------|----------|
| DE 4203456 | A1 | 19930812 | DE 1992-4203456 | 19920207 |
| US 5254711 | A | 19931019 | US 1993-14171 | 19930205 |
| JP 06122667 | A2 | 19940506 | JP 1993-18562 | 19930205 |
| JP 3241472 | B2 | 20011225 | | |

PRIORITY APPLN. INFO.: DE 1992-4203456 A 19920207

OTHER SOURCE(S): CASREACT 119:270685

AB The title process comprises condensation of isophorone with HCN in a 2-stage flow reactor system comprising an initial stage wherein complete mixing is provided and a second stage wherein mixing is suppressed. Thus, operation at 150° in both stages gave 96.5% the title compound

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L9 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:652567 CAPLUS

DOCUMENT NUMBER: 119:252567

TITLE: Process for the preparation of 3-cyano-3,5,5-trimethylcyclohexanone

INVENTOR(S): Woodbury, Richard P.; Thunberg, Jon C.; Vankouwenberg, Steven P.; Begonis, Walter B.

PATENT ASSIGNEE(S): Hampshire Chemical Corp., USA

SOURCE: U.S., 10 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| US 5235089 | A | 19930810 | US 1992-843867 | 19920227 |
| AU 9333783 | A1 | 19930902 | AU 1993-33783 | 19930225 |
| AU 660765 | B2 | 19950706 | | |
| CA 2090555 | AA | 19930828 | CA 1993-2090555 | 19930226 |
| EP 558332 | A1 | 19930901 | EP 1993-301451 | 19930226 |
| EP 558332 | B1 | 19960529 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, PT, SE | | | | |
| JP 06016612 | A2 | 19940125 | JP 1993-61314 | 19930226 |
| AT 138642 | E | 19960615 | AT 1993-301451 | 19930226 |
| ES 2088225 | T3 | 19960801 | ES 1993-301451 | 19930226 |

PRIORITY APPLN. INFO.: US 1992-843867 19920227

AB The title process giving title compound with high yield and low impurity comprises reacting isophorone with HCN in the presence of LiCN catalyst at 80-115° while maintaining the HCN at a controlled rate (to prevent the generation of free LiOH, diisophorone, its nitrile derivs., and HCN polymer); and adding an acid selected from malic acid, oxalic acid, sulfuric acid, and phosphoric acid to precipitate the Li salt.

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LiCN

(FILE 'HOME' ENTERED AT 15:09:39 ON 17 JUN 2004)

FILE 'REGISTRY' ENTERED AT 15:10:00 ON 17 JUN 2004

L1 1 S ISOPHORONENITRILE/CN
L2 1 S ISOPHORONE/CN

CaO

FILE 'CASREACT' ENTERED AT 15:13:02 ON 17 JUN 2004

L3 STRUCTURE UPLOADED
 L4 0 S L3
 L5 0 S L3 FULL

FILE 'CAPLUS' ENTERED AT 15:15:24 ON 17 JUN 2004

L6 88 S L1
 L7 2508 S L2
 L8 28 S L6 AND L7
 L9 18 S L8 AND (HCN OR HYDROGEN CYANIDE)
 L10 7 S L9 AND ?OXIDE

=> s L10 and (BET or Brunauer Emett Teller)
 13208 BET
 2375 BRUNAUER
 34 EMETT
 15732 TELLER
 24 BRUNAUER EMETT TELLER
 (BRUNAUER (W) EMETT (W) TELLER)
 L11 1 L10 AND (BET OR BRUNAUER EMETT TELLER)

=> d L11

L11 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
 AN 2004:386596 CAPLUS
 DN 140:391385
 TI Regioselective hydrocyanation process for the calcium oxide
 -catalyzed preparation of isophorone nitrile from hydrogen
 cyanide and isophorone
 IN Kunsmann-Keitel, Dagmar; Braun, Gerold; Muenster, Ingo; Mundinger, Klaus;
 Scherhag, Gunter; Siegel, Wolfgang
 PA BASF Aktiengesellschaft, Germany
 SO Eur. Pat. Appl., 5 pp.
 CODEN: EPXXDW
 DT Patent
 LA German
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|------------------|----------|
| PI | EP 1418172 | A2 | 20040512 | EP 2003-25652 | 20031107 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| | DE 10251680 | A1 | 20040519 | DE 2002-10251680 | 20021107 |
| | JP 2004155785 | A2 | 20040603 | JP 2003-375444 | 20031105 |
| | US 2004092761 | A1 | 20040513 | US 2003-701513 | 20031106 |
| PRAI | DE 2002-10251680 | A | 20021107 | | |

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L11 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2004:386596 CAPLUS
 DOCUMENT NUMBER: 140:391385
 TITLE: Regioselective hydrocyanation process for the calcium
 oxide-catalyzed preparation of isophorone
 nitrile from hydrogen cyanide and
 isophorone
 INVENTOR(S): Kunsmann-Keitel, Dagmar; Braun, Gerold; Muenster,
 Ingo; Mundinger, Klaus; Scherhag, Gunter; Siegel,
 Wolfgang

PATENT ASSIGNEE(S) : BASF Aktiengesellschaft, Germany
SOURCE: Eur. Pat. Appl., 5 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|----------|
| EP 1418172 | A2 | 20040512 | EP 2003-25652 | 20031107 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| DE 10251680 | A1 | 20040519 | DE 2002-10251680 | 20021107 |
| JP 2004155785 | A2 | 20040603 | JP 2003-375444 | 20031105 |
| US 2004092761 | A1 | 20040513 | US 2003-701513 | 20031106 |

PRIORITY APPLN. INFO.: DE 2002-10251680 A 20021107
AB A regioselective hydrocyanation process for the calcium **oxide**
-catalyzed preparation of isophorone nitrile from **hydrogen**
cyanide and isophorone is presented in which the calcium
oxide regioselective hydrocyanation catalyst has a **BET**
surface area of >1.5 m²/g.